Monte Carlo Methods & MCNP Code Development

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Fast desktop computers and Linux clusters are helping to make Monte Carlo the tool of choice for reactor and radiation transport calculations. General 3D geometry and continuous-energy physics data simplify the detailed modeling of today's complex systems. The increased use of Monte Carlo in recent years has spawned numerous R&D efforts to extend the capabilities of standard production codes. A number of recent advances in Monte Carlo for reactor physics calculations are summarized.

MCNP5 is a general-purpose 3D Monte Carlo code used for neutron, photon, and electron transport. Continued support for MCNP provides opportunities for advanced development in many areas, including:

- Parallel calculations on Linux clusters and ASC teraflop systems
- Stationarity detection and dominance ratio for eigenvalue calculations
- Automated variance reduction for MCNP with deterministic adjoint calculations
- Proton radiography simulation, for beams in the GeV range
- Continuous spatial variations in material properties and tallies

Outline

- Perspective
- Recent Monte Carlo Developments
- MCNP5

Perspective

- **Fast desktop computers**

1980s super:	200 MHz	16 MB	10 GB	\$ 20 M
Today, PC:	2000 MHz	1000 MB	100 GB	\$ 2 K

- **Linux clusters + MPI**
  - **Cheap parallel computing**
  - **Everyone can do parallel computing, not just national labs**

- **Mature Monte Carlo codes**
  - **MCNP, VIM, KENO, MCBEND, MONK, COG, TORT, RACER, RCP, …**

- **New generation of engineers/scientists**
  - **Less patience for esoteric theory & tedious computing procedures**
  - **Computers are tools, not to be worshipped**
  - **What's a slide rule ???**

➜ More calculations with Monte Carlo codes

Perspective

- As computing power has increased, the use of Monte Carlo methods for reactor analysis has grown
- Also, since more histories give better localized statistics, the principal uses of Monte Carlo have evolved:

1960s:	K-effective
1970s:	K-effective, detailed assembly power
1980s:	K-effective, detailed 2D whole-core
1990s:	K-effective, detailed 3D whole-core
2000s:	K-effective, detailed 3D whole-core, depletion, reactor design parameters

➜ Recent Monte Carlo R&D is focussed on advanced methods for modeling & design parameters

- Source-shape Effect on Perturbations
- Pebble-bed Reactor Modeling
- Stationarity Diagnostics
- Dominance Ratio
- Beta-effective Calculation
- Continuous Materials & Tallies
- Automated Variance Reduction
- Monte Carlo Depletion
- Point KENO-Va
- International Handbook of Evaluated Criticality Benchmark Experiments

- Work by

  Yasunobu Nagaya (JAERI)

- Reported in

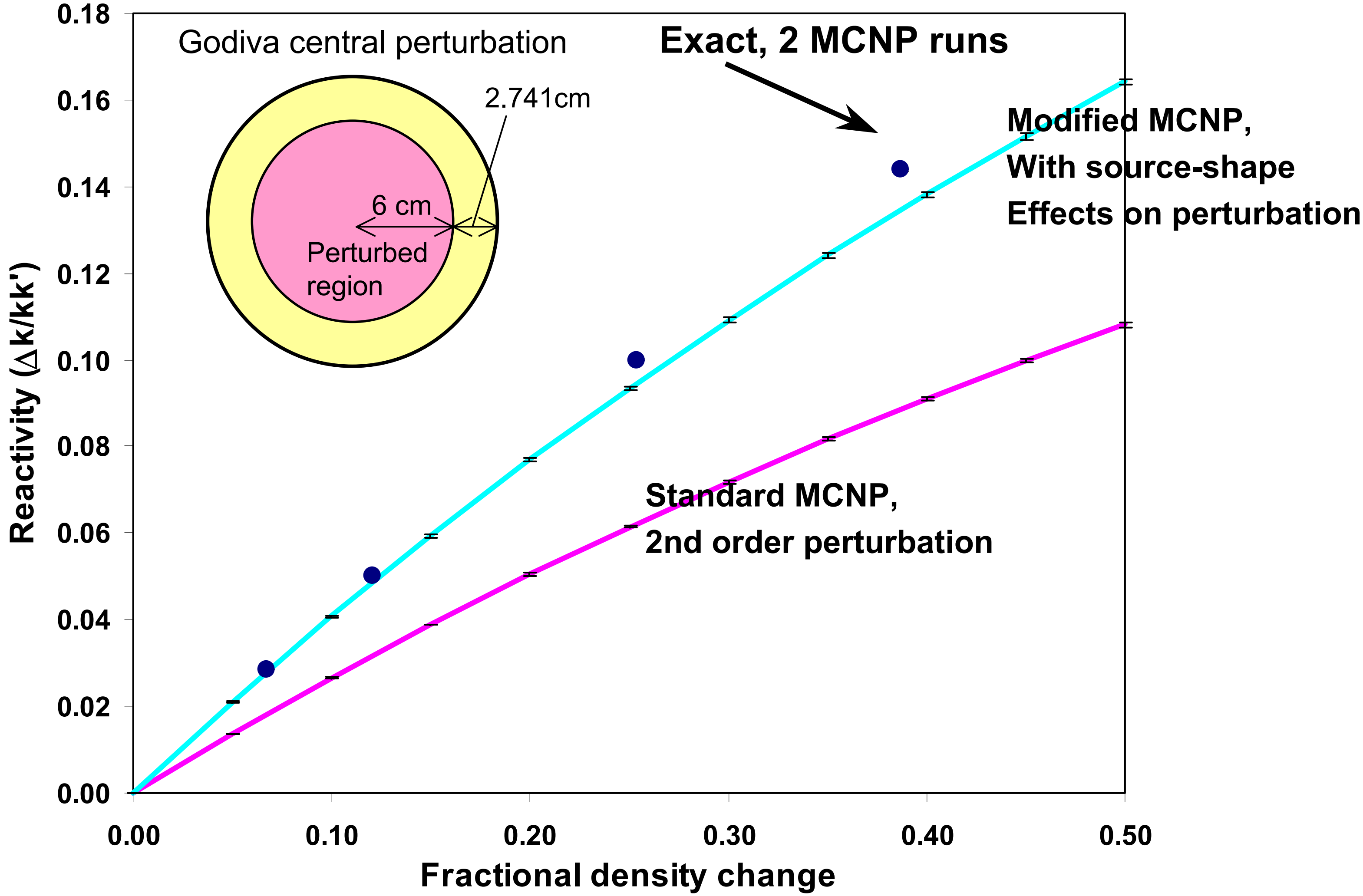
  Y.Nagaya & T.Mori, “Evaluation of Perturbation Effect Due to Fission-Source Change in Eigenvalue Problems by Monte Carlo Methods,” PHYSOR-2000 (2000).

  Y. Nagaya & F.B. Brown, "Estimation of Change in Keff due to Perturbed Fission Source Distribution in MCNP", M&C Topical, Gatlinburg (2003)

  Y. Nagaya & F.B. Brown, "Implementation of a Method to Estimate Change in Eigenvalue Due to Perturbed Fission Source Distribution into MCNP", LA-UR-03-1387 (2003).

- MCNP & other Monte Carlo codes assume that the fission source distribution does not change when a perturbation is introduced.
- This approximation can lead to significant errors in perturbation theory estimates
- Accounting for source-shape changes in Monte Carlo perturbation theory can be an important effect

Central perturbation



- Work by

  Malcom Armishaw, Nigel Smith, Edmund Shuttleworth
  (Serco Assurance, Winfrith)

- Reported in

  "Particle Packing Considerations for Pebble Bed Fuel Systems", ICNC-2003 proceedings, JAERI-Conf-2003-019 (2003)

- Multiple levels of heterogeneity represented explicitly, using MONK "hole geometry"

- Several algorithms for random placement & packing of spheres

- Provides evidence that packing schemes can have a significant effect on Keff, & that simple lattice approaches may not be adequate

Pebble-bed Reactor Modeling

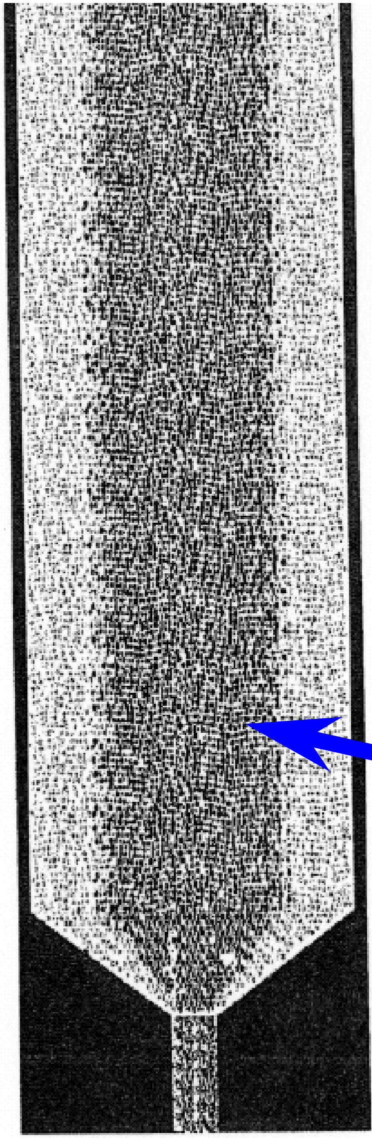


Fig. 3 PBMR hole packing spheres into a reactor core.

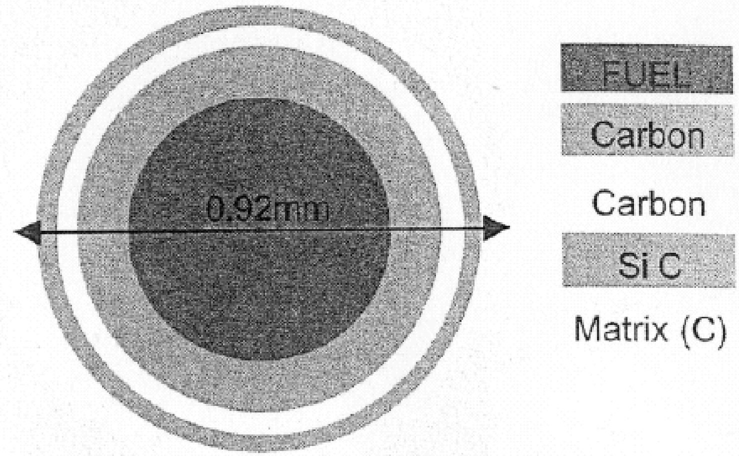


Fig. 4 A fuel grain defined using the PEBBLE hole.

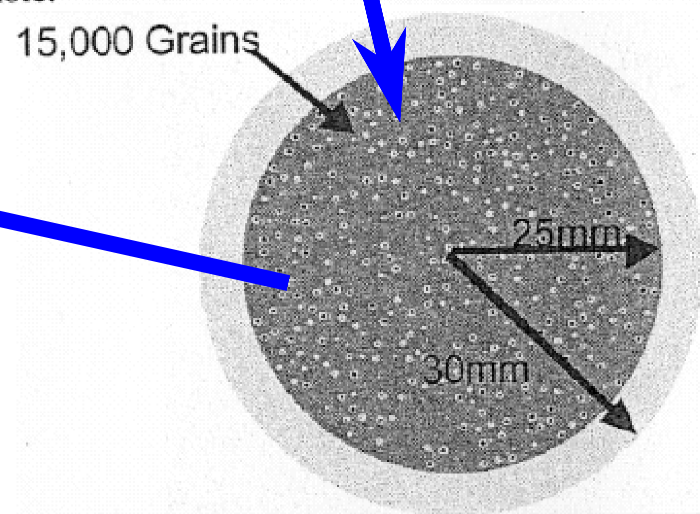


Fig. 5 A pebble defined using the PEBBLE hole.

Stationarity Diagnostics

- **Work by**

  Taro Ueki (Univ. New Mexico), Forrest Brown (LANL)

- **Reported in**

  T Ueki, "**Intergenerational Correlation in Monte Carlo K-Eigenvalue Calculations**", LA-UR-02-0190, Nucl. Sci. Eng. (2002)

  T Ueki & FB Brown, "**Autoregressive Fitting for Monte Carlo K-effective Confidence Intervals**", LA-UR-01-6770, Trans ANS (June 2002)

  T Ueki & FB Brown, "**Stationarity Diagnostics Using Shannon Entropy in Monte Carlo Criticality Calculations I: F Test**", LA-UR-02-3783, Trans ANS (Nov 2002)

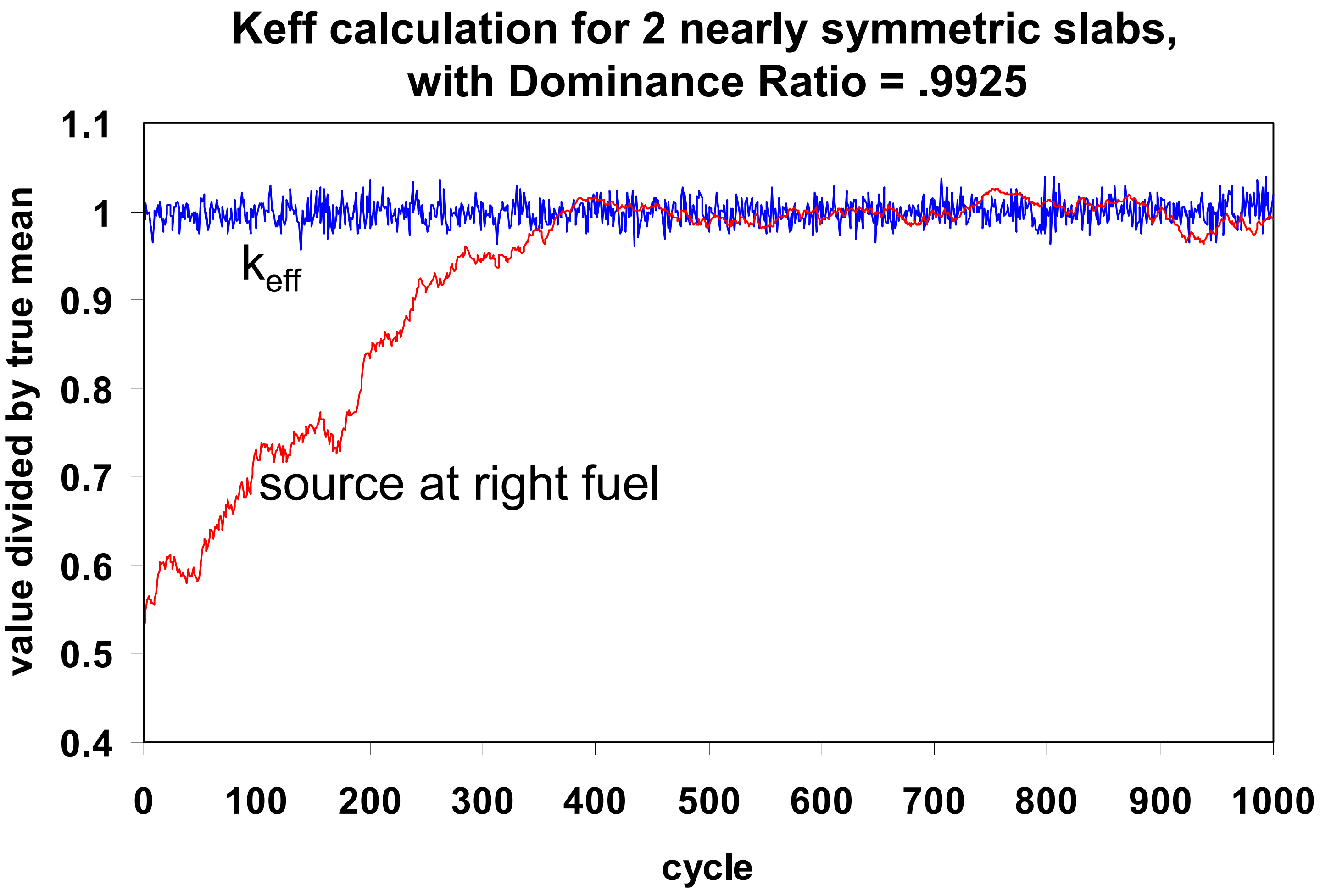
  T Ueki & FB Brown, "**Stationarity and Source Convergence in Monte Carlo Criticality Calculations**", LA-UR-02-6228, ANS M&C Topical Meeting (April, 2003)

- **In a series of related papers, the theory of Monte Carlo eigenvalue calculations has been significantly extended, explicitly accounting for correlation effects**

- **First real progress in this area since Gelbard & Prael (1970s) and Brissenden & Garlick (1980s)**

- **Relative entropy of the fission source distribution was shown to be an effective diagnostic for stationarity**

- Keff is an integral quantity - converges faster than source shape



- **Shannon entropy of the source distribution tallies has been found to be a good measure of convergence & stationarity**
- **Relative entropy is used in practice**

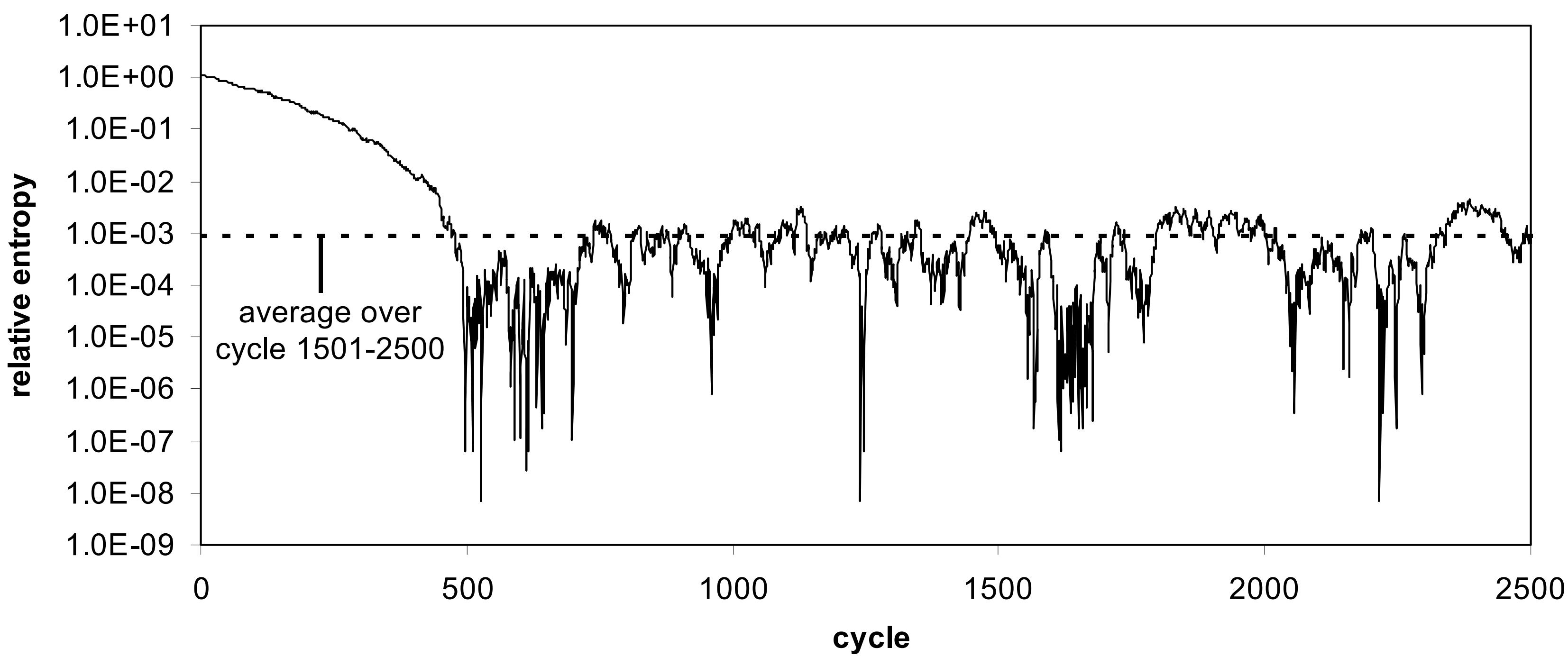
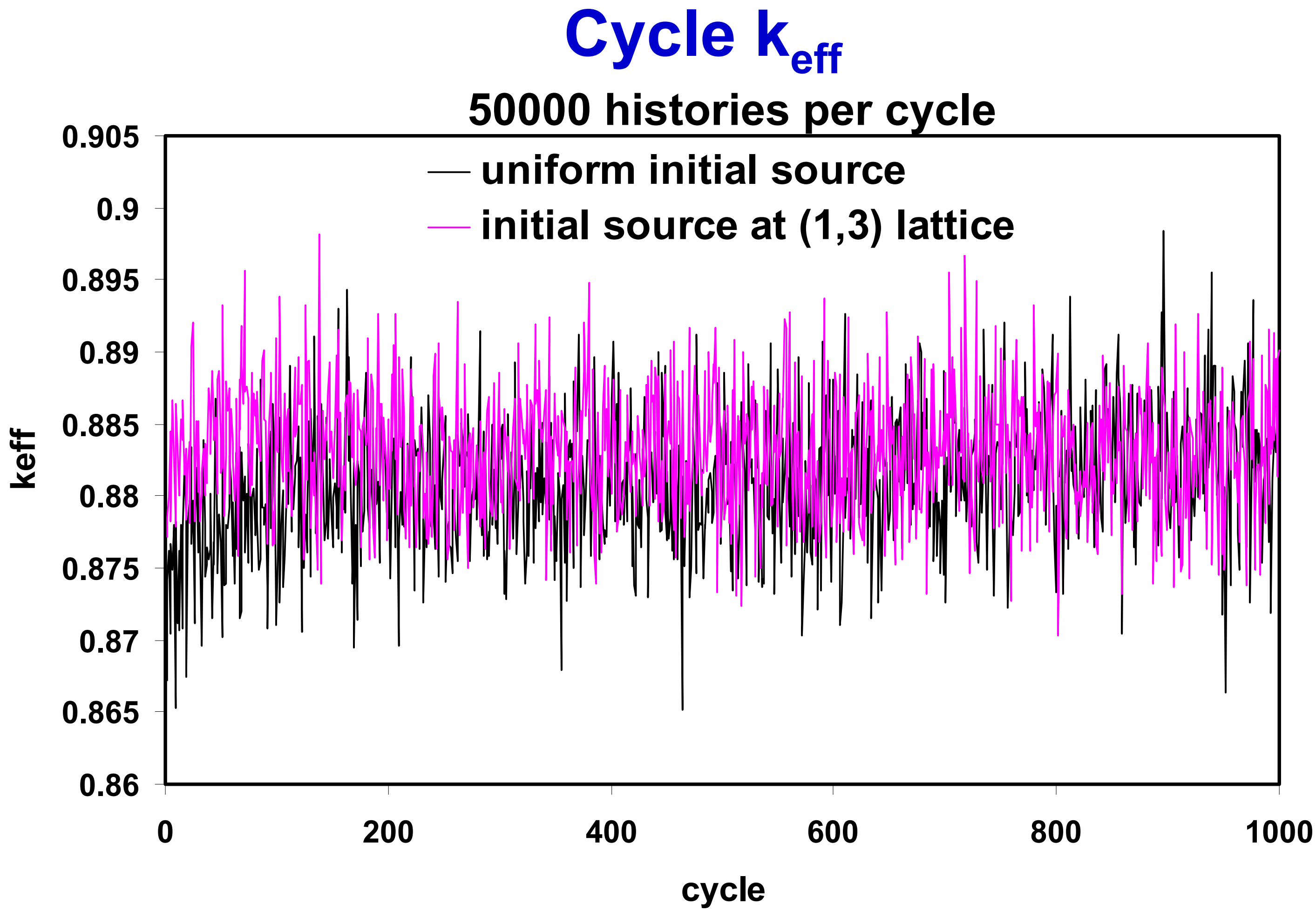


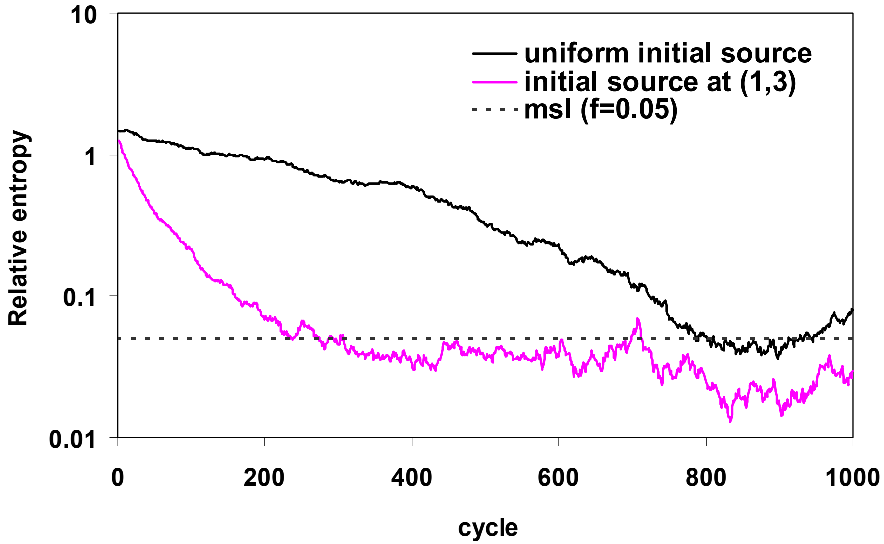
Figure 3: Posterior computation of relative entropy assuming the true source is the mean source over 1501-2500 cycles (problem 1)

- **Plots of single-cycle Keff or cumulative Keff are difficult to interpret when assessing convergence**

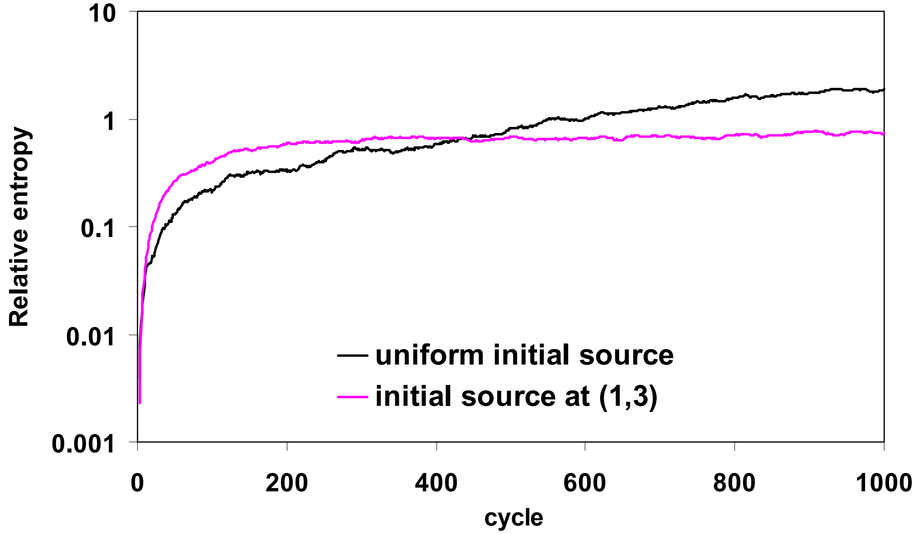


Stationarity Diagnostics

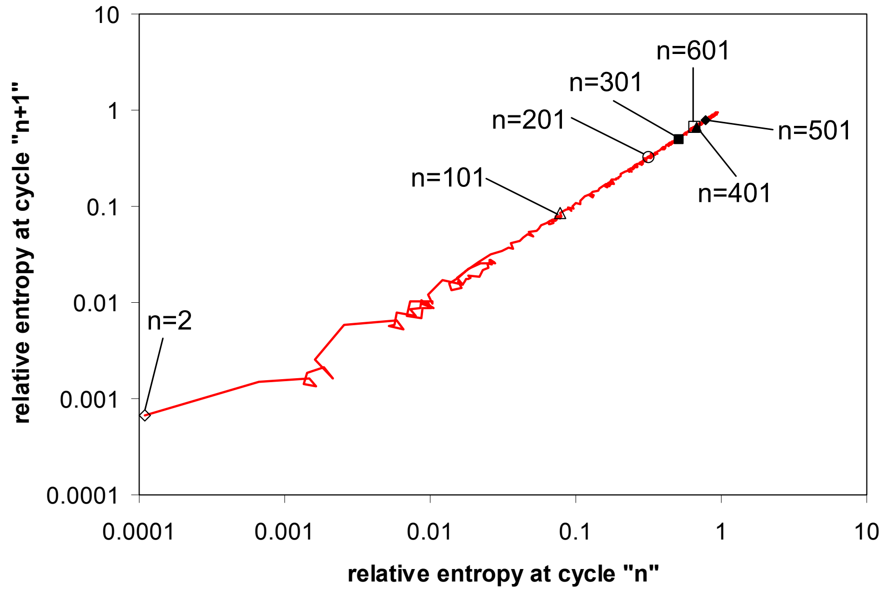
Posterior relative entropy
(500 inactive and 500 active cycles)



Progressive relative entropy



One-cycle delay embedding plot of relative entropy wrt initial source



Dominance Ratio

- **Work by**

  Taro Ueki (Univ. New Mexico), Forrest Brown (LANL)

- **Reported in**

  T Ueki, FB Brown, DK Parsons, "**Dominance Ratio Computation via Time Series Analysis of Monte Carlo Fission Sources**" , LA-UR-03-0106, Trans ANS (June 2003)

  T Ueki, FB Brown, DK Parsons, & DE Kornreich, "**Autocorrelation and Dominance Ratio in Monte Carlo Criticality Calculations**", LA-UR-02-5700, Nucl. Sci. Eng. (Nov, 2003)

  T Ueki, FB Brown, DK Parsons, JS Warsa, "**Time Series Analysis of Monte Carlo Fisison Sources: I. Dominance Ratio Calculation**", LA-UR-03-5823, submitted to Nucl. Sci. Eng.

- **After the source distribution is stationary, time series analysis can produce the dominance ratio (K_1/K_{eff})**

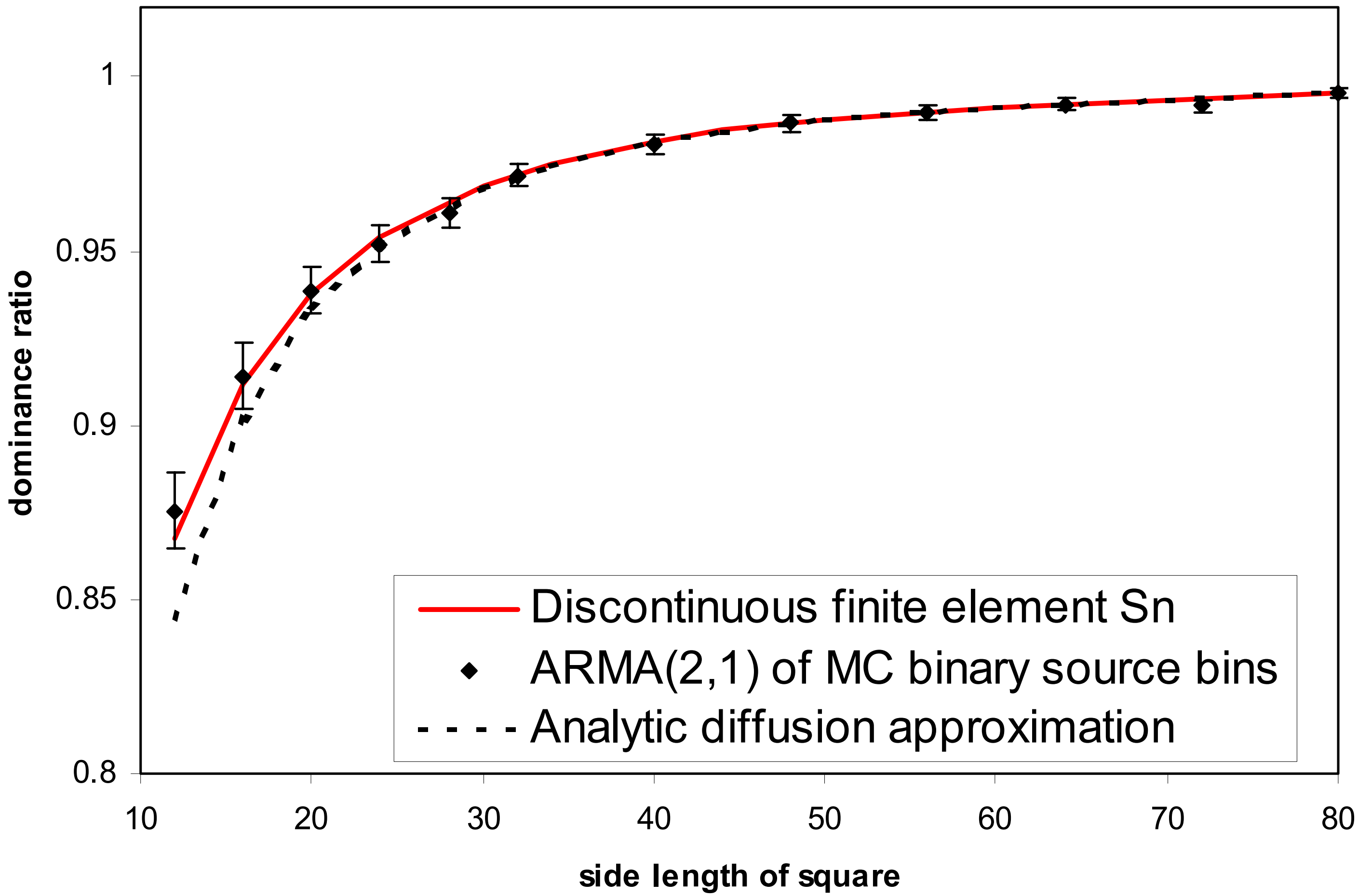
- **This is the first known successful technique for calculating the dominance ratio with a continuous Monte Carlo code**

  Note:

  – MC codes which produce a fission matrix could compute the dominance ratio for the fission matrix. This would approach the dominance ratio of the physical problem as the fission matrix mesh is refined. Usually, computer storage limits prevent such refinement.

  – The present method is not dependent on a mesh, & can yield accurate results for any problem

Dominance ratio of 2D homogeneous square problems (95% (1.96σ) CI)



Beta-effective Calculations

- Work by

  Steven C. van der Marck, Robin Klein Meulekamp
  (NRG, Netherlands)

- Reported in

  "Calculating the effective delayed neutron fraction using Monte Carlo techniques", PHYSOR-2004 (2004)

- Modified MCNP to keep track of fissions induced by prompt & delayed neutrons, β_{eff} = delayed / total

- Can be computed during normal Keff calculation, at essentially zero extra cost

- Results within a few percent of experiment

Continuous Materials & Tallies

- **Work by**

  FB Brown (LANL), WR Martin, D Griesheimer (Univ. Mich)

  D Legrady & JE Hoogenboom (Delft Univ.)

- **Reported in**

  FB Brown, D Griesheimer, & WR Martin, **"Continuously Varying Material Properties and Tallies for Monte Carlo Calculations",** PHYSOR-2004, Chicago, IL (2004)

  FB Brown & WR Martin, **"Direct Sampling of Monte Carlo Flight Paths in Media with Continuously Varying Cross-sections",** ANS Mathematics & Computation Topical Meeting, Gatlinburg, TN (2003).

  DP Griesheimer & WR Martin, **"Estimating the Global Scalar Flux Distribution with Orthogonal Basis Function Expansions",** Trans. Am. Nucl. Soc. 89 (Nov, 2003)

  DP Griesheimer & WR Martin, **"Two Dimensional Functional Expansion Tallies for Monte Carlo Simulations,"** PHYSOR-2004, Chicago, IL (2004)

  D Legrady & JE Hoogenboom, **"Visualization of Space-dependent Responses of Monte Carlo Calculations Using Legendre Polynomials",** PHYSOR-2004, Chicago, IL (2004)

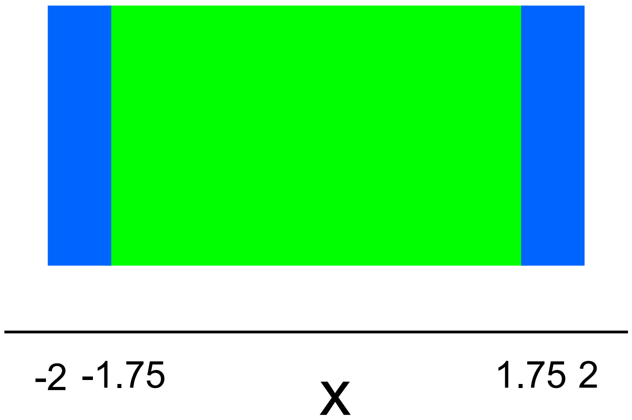
- **Monte Carlo codes such as MCNP5 are continuous in <u>particle properties</u> (position, direction, & energy) and <u>collision physics</u> (energy & angle), but use zero-th order representations of tallies and material properties:**
  - Material properties are assumed constant within each cell
  - Tally bins provide average scores within each cell
- **Using Legendre expansions of material densities & tallies within each cell, Monte Carlo codes can be extended to a <u>continuous treatment of materials & tallies</u>**

Eigenvalue calculation - depleted core with reflector

- **Continuous representation: 5th order Legendre expansion for material density & tallies within each region**

- Density varies quadratically in core: .25 at center, 2.25 at edges

- Constant density in reflector, 1.0



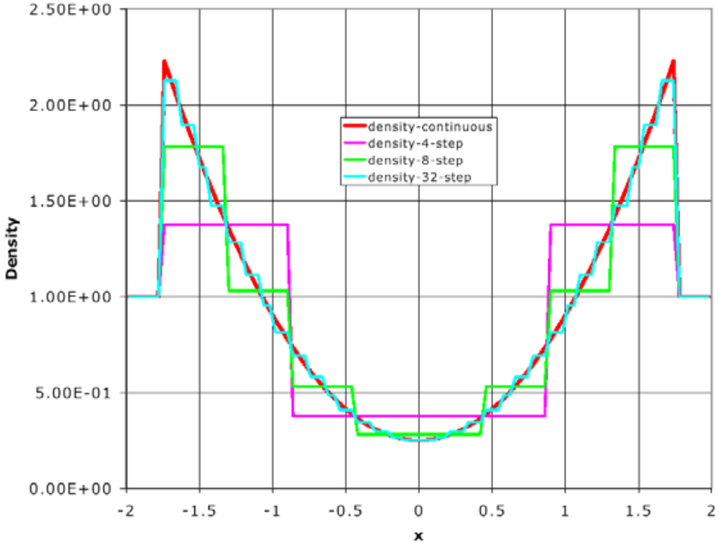


Figure 2. Density variation for Problem B: Quadratic variation for center fissionable region and various stepwise approximations

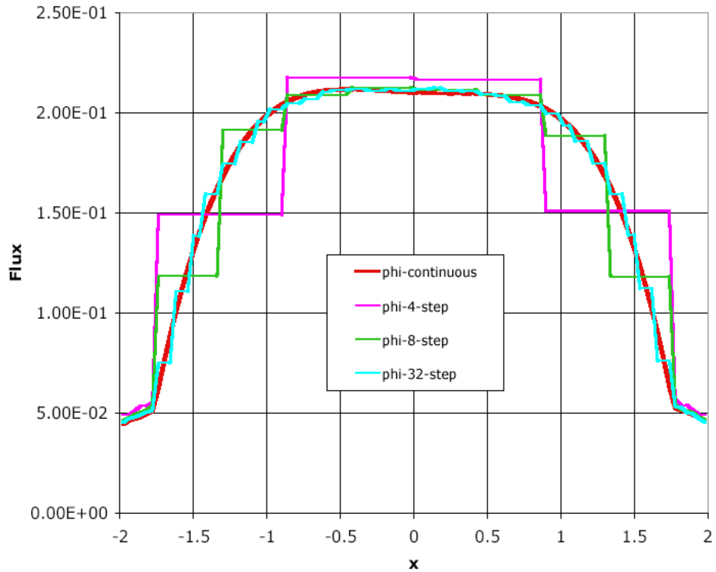


Figure 4. Flux results for Problem B: Quadratic density variation, continuous tallies and various stepwise approximations

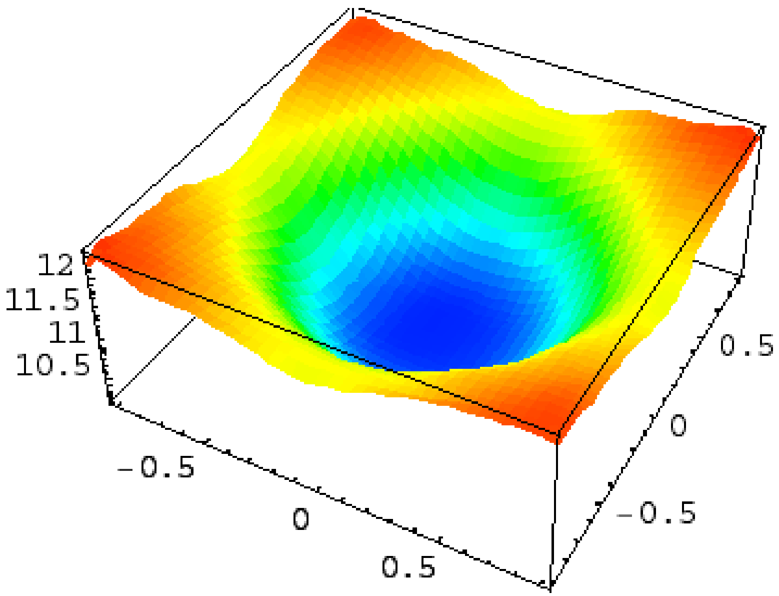


Figure 2a. 9x9 Legendre expansion tally for thermal neutron flux across the fuel pin obtained in a 2 million history simulation.

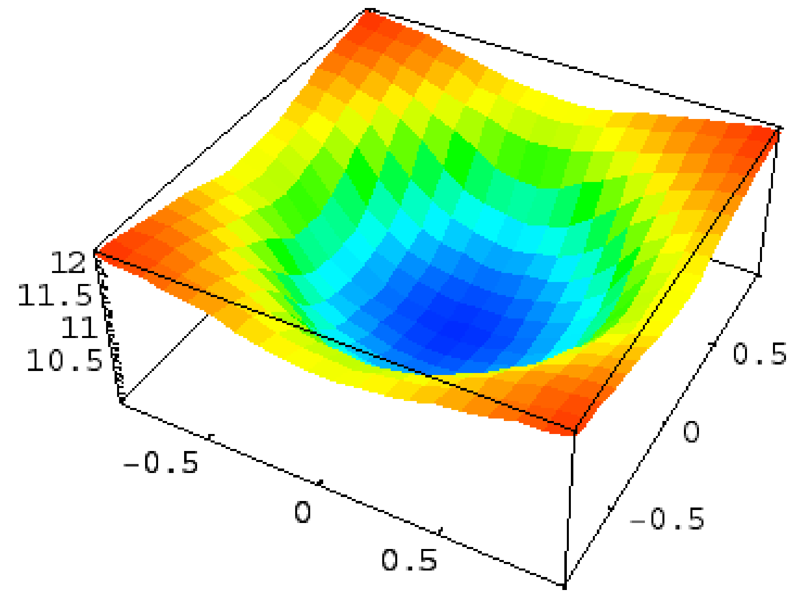


Figure 2b. MCNP5 20×20 mesh tally for thermal neutron flux across the fuel pin obtained in a 2 million history simulation.

- Work by

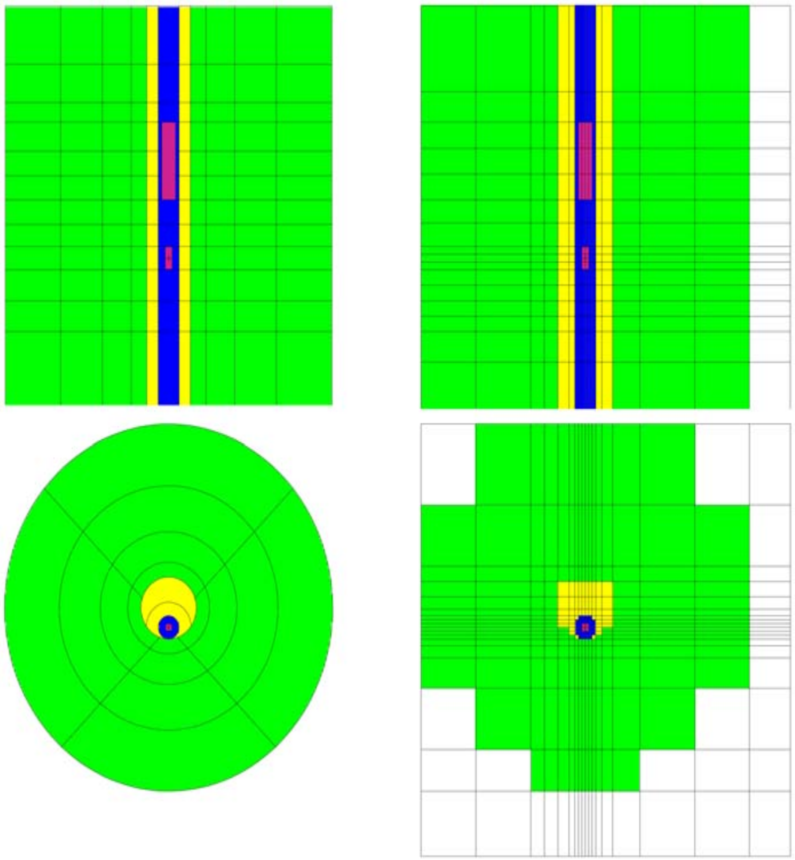
  Wagner (ORNL), Haghighat & students (PSU, UF), Sweezy (LANL), Univ. Texas, & others

- A number of R&D efforts have been underway to use deterministic adjoint calculations to reduce the variance in Monte Carlo calculations
  - Monte Carlo combinatorial geometry is converted to a mesh geometry
  - Deterministic (Sn) calculation of adjoint flux
  - Adjoint fluxes used to generate importance weights for Monte Carlo
  - Monte Carlo calculation using the importance weights to reduce variance (or run-time)

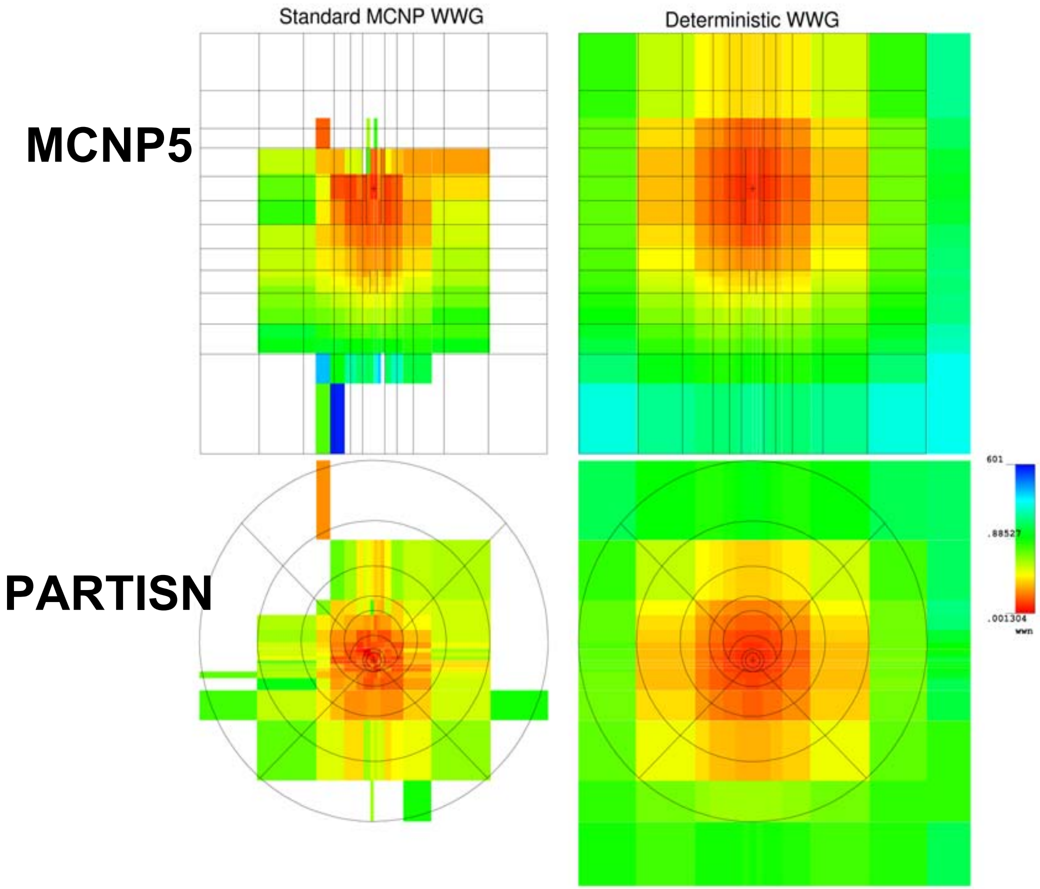
- Example from Sweezy's work at LANL, using adjoint fluxes from PARTISN (3D Sn code) to generate weight windows for MCNP5

Automated Variance Reduction

Geometry



Generated Importances



Run-times for importance generation:

MCNP5 - hours, PARTISN - minutes

Large-scale Monte Carlo Calculations

- **Work by**

  Wolfgang Bernnat (Stuttgart), S Langenbuch, W Zwermann (GRS)

  HJ Shim, BS Han, & CH Kim (Seoul Nat. Univ.)

- **Reported in**

  W. Bernnat, "Coupled Monte Carlo & Burnup Calculations for Reasearch & Power Reactors", SNA-2003, Paris (2003)

  W. Bernatt, S. Langenbuch, W. Zwermann, "Monte Carlo Large Scale Reactor Physics Calculations", SNA-2003, Paris (2003)

  HJ Shim, BS Han, CH Kim, "Numerical Experiment on Variance Biases & Monte Carlo Neutronics Analysis with Thermal Hydraulic Feedback", SNA-2003, Paris (2003)

- **Very impressive, large-scale calculations**
- **Bernnat:**
  - **Monte Carlo calculations of research reactor, including depletion, using modified version of MCNP4C+ORIGEN; 50,000 zones with 100 nuclides/zone, parallel calculations**
  - **Monte Carlo depletion of LWR assemblies & clusters of assemblies**
  - **Detailed 3D Monte Carlo calculations of BWRs**
- **Shim, Han, Kim:**
  - **PWR analysis using Monte Carlo with thermal-hydraulic feedback**
- **Others**
  - **Moderate sized Monte Carlo depletion with MONTEBURNS + MCNP (Trellue, LANL)**

Large-scale Monte Carlo Calculations

Bernnat, SNA-2003

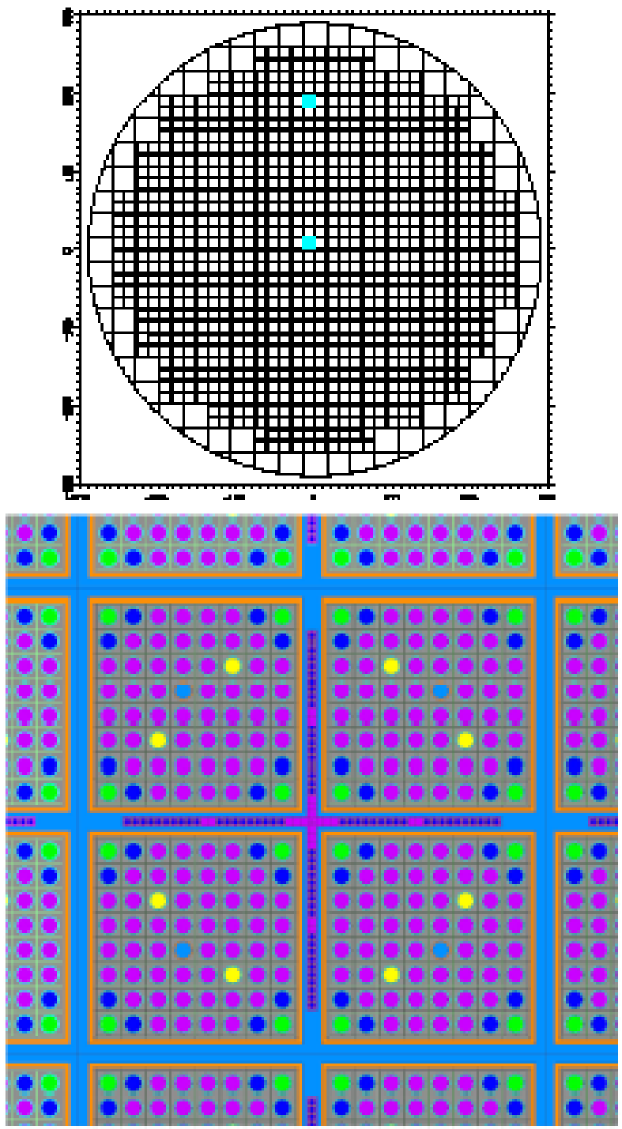


Fig. 1. Horizontal cut through the MCNP model of a 1,300 MW BWR Top: The whole reactor core. Bottom: A four-bundle of fuel assemblies in its surrounding.

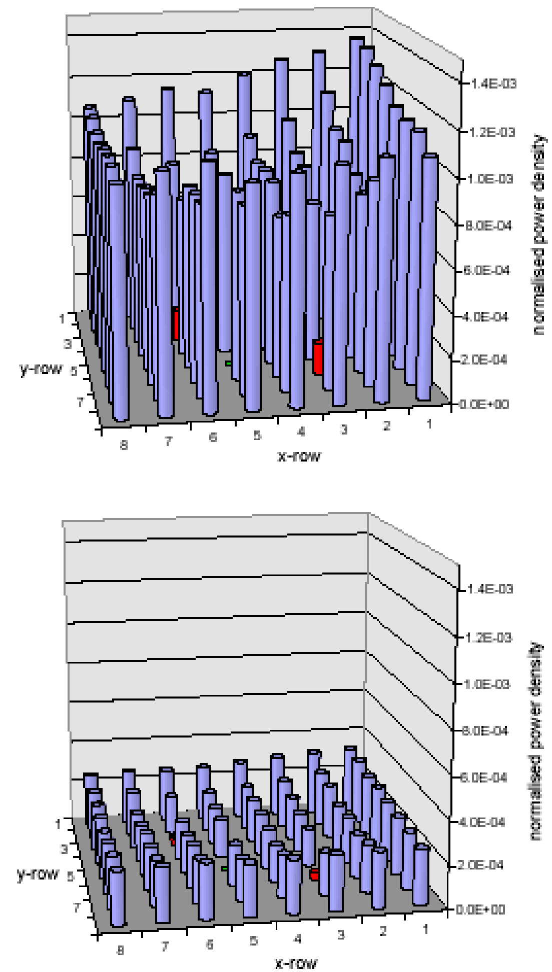


Fig. 11. MCNP results for the pin-wise power distribution in axial fuel assembly sections of 53 cm length located in the central part (upper figure) and near the periphery (lower part) of a large BWR core in cold state; approximately critical control rod pattern. 200.000,000 active particle histories (4,000 generations with 50,000 neutrons/generation). Relative uncertainties are given as 1.3-1.8 % for the central part and 2.6-3.9 % for the interval located near the periphery. (The gadolinium fuel pins are displayed in red, the water pins in green.)

Point KENO-Va

- Work by

  ME Dunn, NM Greene, DF Hollenbach, LM Petrie (ORNL)
- Reported in

  "Point KENO Va: A Continuous-Energy Monte Carlo Code for Criticality Safety Applications", PHYSOR-2004 (2004)

- Provides another continuous-energy Monte Carlo code to compare with MCNP5 (LANL) & VIM (ANL)

- More code comparisons on real benchmark problems benefits all of us - code developers & users

Int. Crit. Safety Benchmark Eval. Project

- Work by
  - J. Blair Briggs (INEEL) & many others
    (US, UK, Japan, Russia, France, Hungary, Korea, Slovenia, Yugoslavia, Kazakhstan, Israel, Spain, OECD-NEA)
  - International Criticality Safety Benchmark Evaluation Project
- Reported in
  - "International Handbook of Evaluated Criticality Benchmark Experiments", OECD Nuclear Energy Agency, NEA/NSC/DOC(95)03 (updated yearly on CD)

- Extensive compilation of criticality benchmark experiments, with detailed descriptions, measured results, estimated tolerances
- Benchmark specifications for 2881 critical, near critical, or subcritical configurations
- 330 evaluations, 24,000 pages in 7 volumes
- All entries have been carefully reviewed & evaluated

- **Verification & validation effort for MCNP makes use of 31 cases taken from the *International Handbook of Evaluated Criticality Benchmark Experiments***
- **Wide variety of fissile materials, configurations, & spectra:**

Spectrum	Fast			Intermediate	Thermal	
Geometry	Bare	Heavy Reflector	Light Reflector	Any	Lattice of Fuel Pins in Water	Solution
^{233}U	Jezebel-233	Flattop-23	U233-MF-05 (2)*	Falstaff (1)†	SB-2½	ORNL-11
HEU	Godiva Tinkertoy-2 (c-11)	Flattop-25	Godiver	Zeus (2) UH_3 (6)	SB-5	ORNL-10
IEU	IEU-MF-03	BIG TEN	IEU-MF-04	Zebra-8H‡	IEU-CT-02 (3)	STACY-36
LEU					B&W XI (2)	LEU-ST-02 (2)
Pu	Jezebel Jezebel-240 Pu Buttons (3)	Flattop-Pu THOR	Pu-MF-11	HISS/HPG‡	PNL-33	PNL-2

* Numbers in parentheses identify a specific case within a sequence of benchmarks
† Extrapolated to critical
‡ k_∞ measurement

HEU-MET-THERM-003

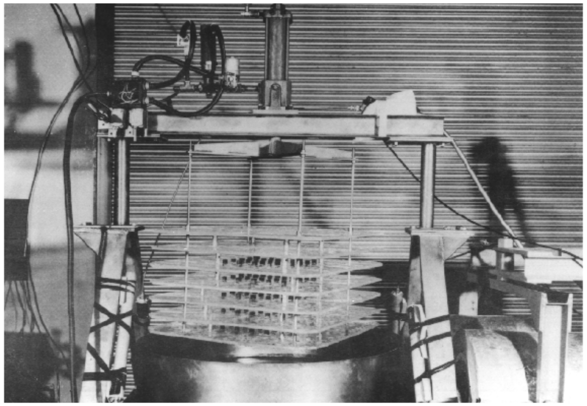
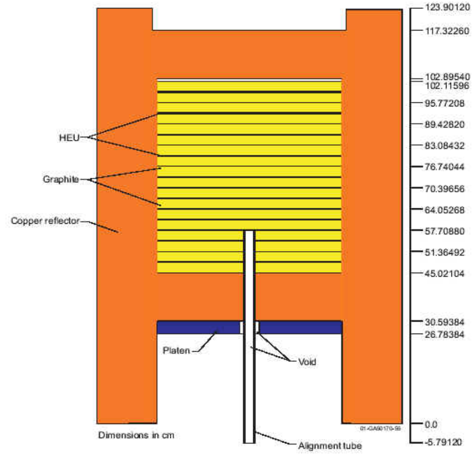
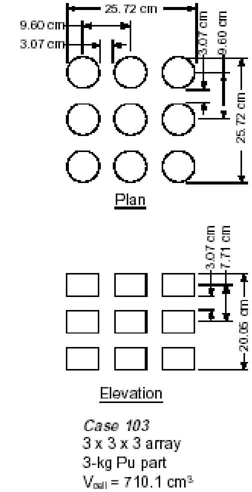


Figure 2. Array of 0.5-in. Cubes Prior to Immersion.

Zeus-2, HEU-MET-INTER-006, case 2



PU-MET-FAST-003, case 3



IEU-COMP-THERM-002, case 3

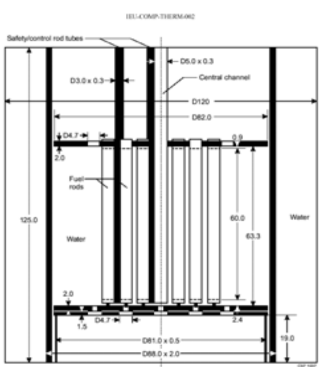
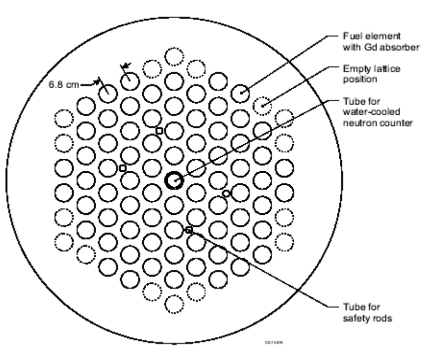


Figure 9. Model of Core

IEU-COMP-THERM-002



...e 6. Lattice Plate Loading Chart for Assemblies with Gd Absorber (Case 3 and Case 4).

PNL-33 - MIX-COMP-THERM-002

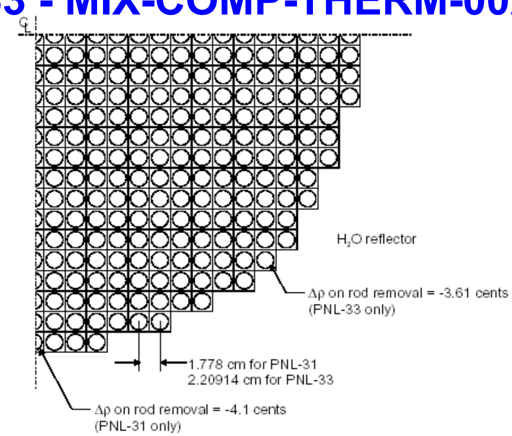
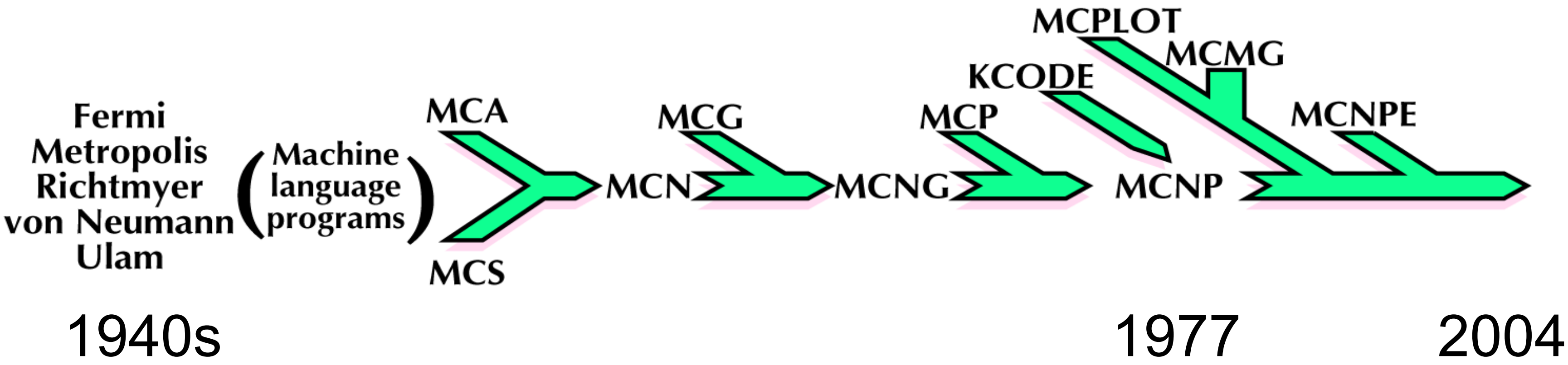


Figure 7. Fuel Loading for PNL-31 and PNL-33.

MCNP5

Forrest Brown, Tom Booth , Jeffrey Bull, Art Forster,
Tim Goorley, Grady Hughes, Russell Mosteller, Richard Prael,
Elizabeth Selcow, Avneet Sood, Jeremy Sweezy,
Susan Post, Richard Barrett



- **Monte Carlo transport of neutrons, photons, & electrons**
  - **General 3D geometry**
  - **Continuous-energy physical data**
  - **Many code options: Keff, detectors, variance reduction, tallies, …**
- **For more than 25 years, MCNP & its data libraries have been developed and supported by the Monte Carlo team in X-Division (and its predecessors)**
  - **Continued strong support for MCNP provides funding for R&D activities in many diverse areas of Monte Carlo methods**

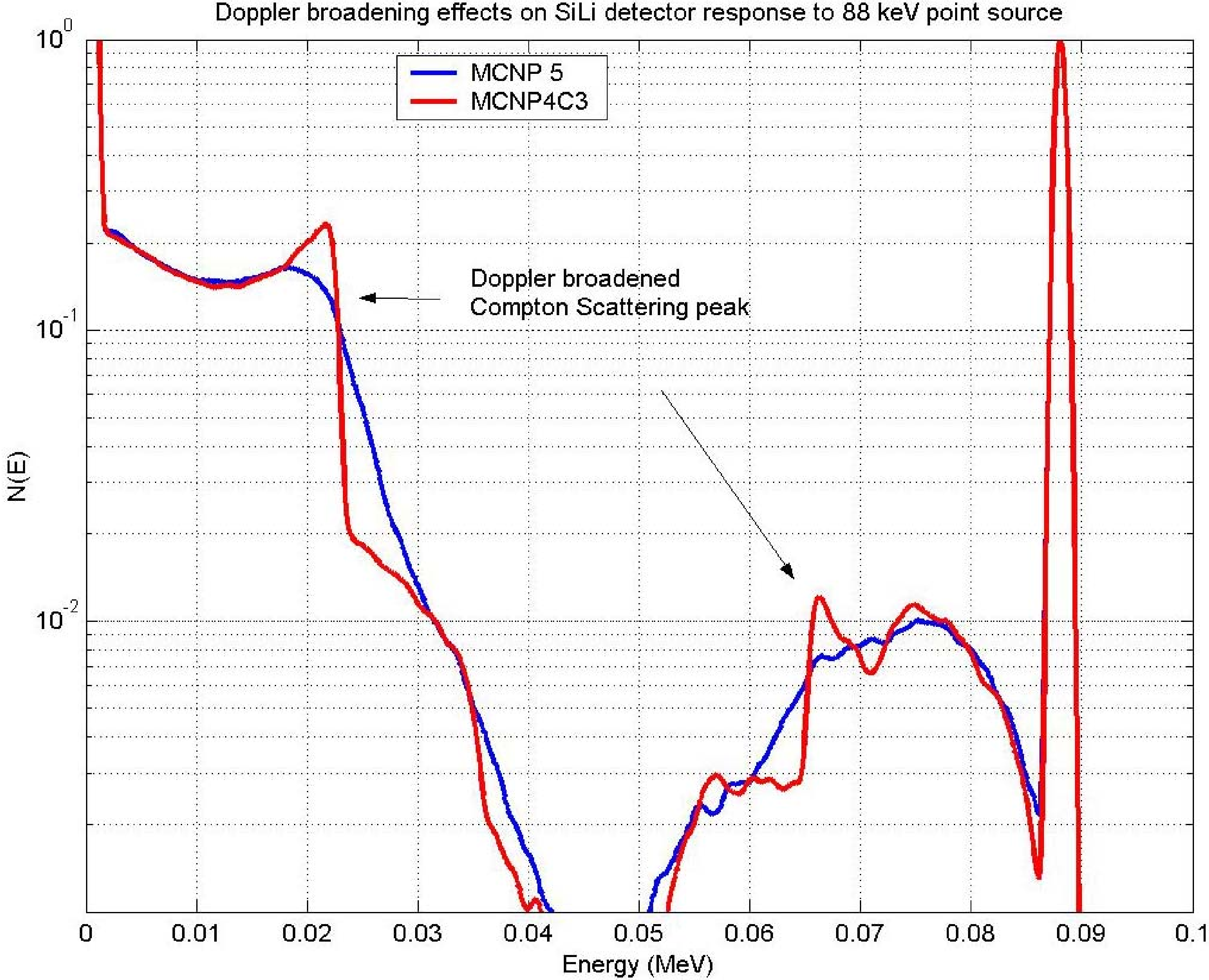
During 2001-2002, every line of MCNP coding was reworked to produce MCNP5

- Conversion to ANSI-Standard Fortran-90
- Emphasis on code readability & ease of future development
- Standard parallel coding: MPI (message-passing) + OMP (threads)
- Vastly improved modern coding style
- Fortran-90 dynamic memory allocation
- Completely new installation system
- New features & new physics
- Extensive SQA and V&V

New Features in MCNP5

- Updated MCNP Users Manual – 1,000 pages
- Doppler Energy Broadening for Photon Transport
- Extended Random Number Package
- Improved Parallel Processing
- Mesh Tallies
- Image Tallies, radiographs
- Sources: translate/rotate/repeat, Gaussian, particle type
- Easier specification of sources in repeated structures
- Time & energy splitting/rouletting
- Unix-based build system, using GNU make
- Plotting improvements
- Pulse height tally variance reduction (Fall, 2004)

Doppler Energy Broadening for Photons



New Data Libraries

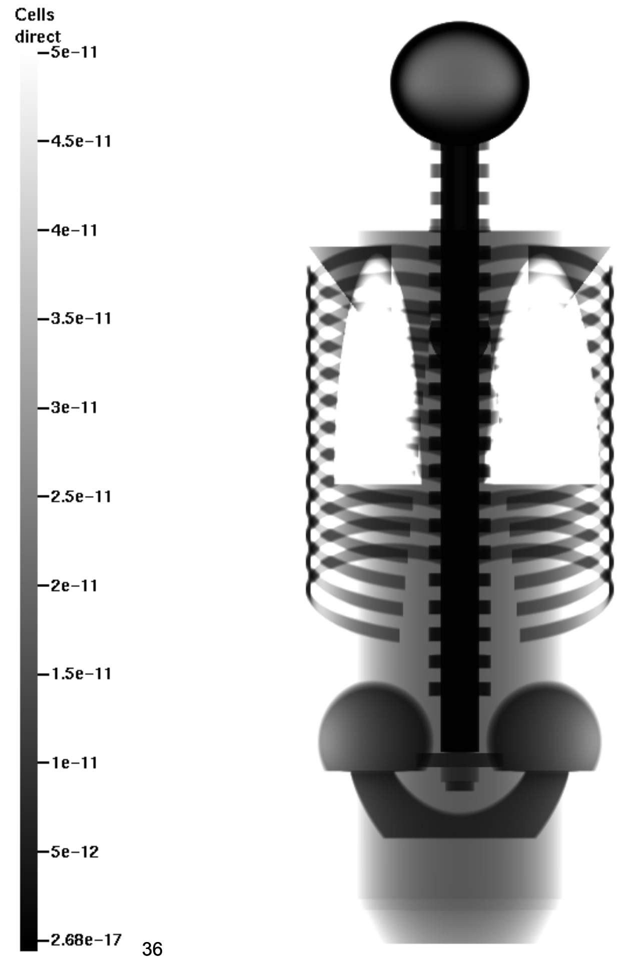
- **New data libraries released by X-5 Data Team**
  - **ENDF66**: Based on ENDF/B-VI, Release 6
  - **ACTI**: Based on ENDF/B-VI, Release 8
  - **SAB2002**: Improved evaluations for thermal scattering
  - **MCPLIB03** & **MCPLIB04**: New photoatomic data libraries
- **ENDF66**
  - **173 nuclides**, compared with 122 nuclides for ENDF60
  - Smaller NJOY processing tolerance, 0.001 instead of ~0.005
  - Probability tables, charged-particle production, delayed neutron data
  - Tabular angular distributions
- **ACTI**
  - MCNP data for prompt gamma-ray spectroscopy, includes **41 nuclides**
  - Advanced Computational Technology Initiative (ACTI) CRADA
- **SAB2002**
  - Based on ENDF/B-V1.3
  - Data for **15 moderators**, includes more secondary energies and angles

Neutral Particle Image Tallies

- Neutron and photon radiography uses a grid of point detectors (pixels)
- Each source and collision event contributes to all pixels

MCNP Model of Human Torso

Simulated Radiograph – 1 M pixels

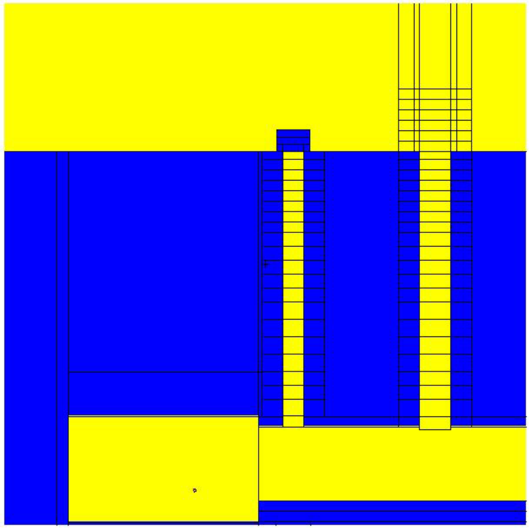


Proton Storage Ring
at LANSCE accelerator

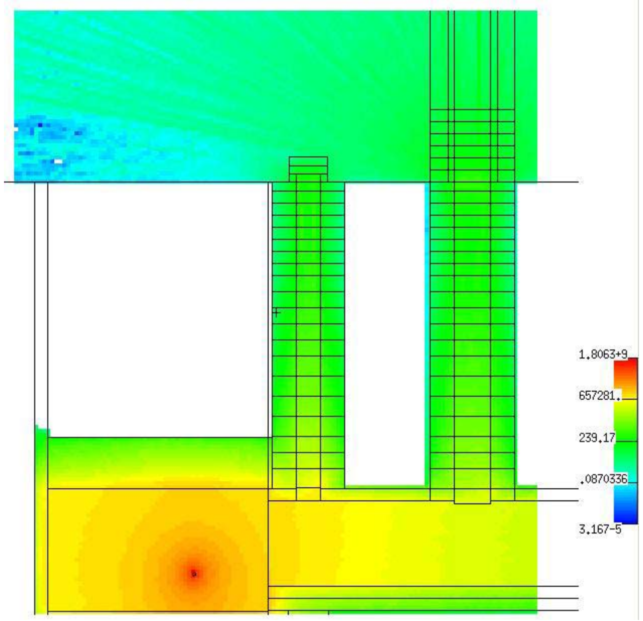
Geometry

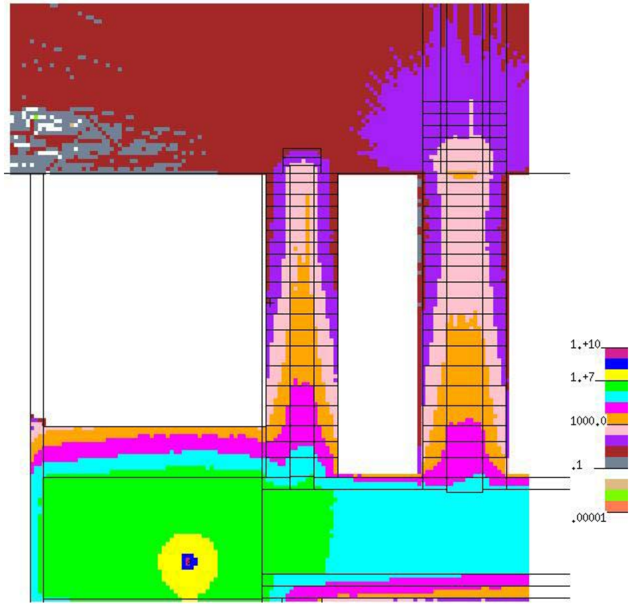
Blue = concrete

Yellow = air



Dose rate calculation for cable penetrations





Computer Systems Supported

Serial & parallel (MPI, OMP, MPI/OMP, PVM, PVM/OMP):

- Unix systems
  - SGI IRIX64
  - IBM AIX
  - HP/Compaq OSF1
  - Sun SunOS

Serial & parallel (MPI, PVM):

- Linux systems
  - with Absoft compiler
  - with Lahey compiler
  - with Intel compiler
  - with Portland Group compiler
  - with NAG compiler
- Mac OS X systems
  - with Absoft compiler
  - with IBMXL compiler

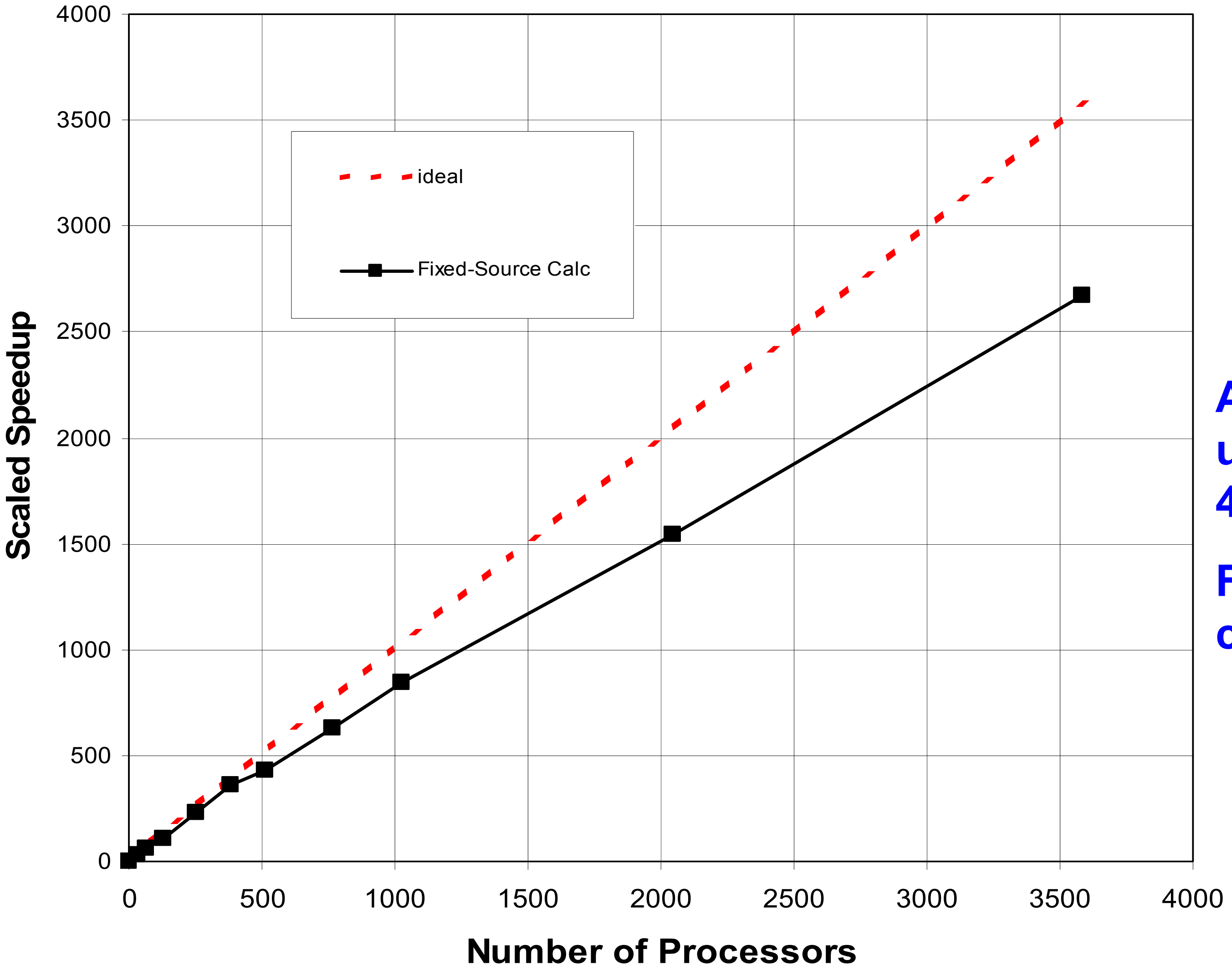
Serial & parallel (MPI, PVM):

- Windows PC systems
  - with CVF compiler
  - with Absoft compiler
  - with Lahey compiler
  - with Intel compiler

- Itanium systems
  - with Intel compiler

X11 graphics – all systems

MCNP5 Parallel Scaled Speedup



ASCI Q system, using MPI+OpenMP, 4 threads/MPI-task

Fixed-source calculation

www-xdiv.lanl.gov / x5 / MCNP

- **Has all recent LA-UR reports & publications:**
  - New version of criticality primer (~200 pages):
    "**Criticality Calculations with MCNP5 - A Primer**", LA-UR-04-0294
  - "**MCNP — A General Monte Carlo N-Particle Transport Code, Version 5, Volume I: Overview and Theory**", LA-UR-03-1987
  - **"Bibliography of MCNP Verification & Validation: 1990-2003",** LA-UR-03-9032
  - All **Ueki/Brown papers** on k-effective calculations:
    correlation effects, stationarity diagnostics, dominance ratio, etc.
  - "**MCNP5 Parallel Processing Workshop**", LA-UR-03-2228,
    parallel Monte Carlo, Linux clusters, Windows clusters
  - … and many more
- **MCNP5 updates & patches**
- **Schedule for upcoming MCNP5 classes**

Work in progress

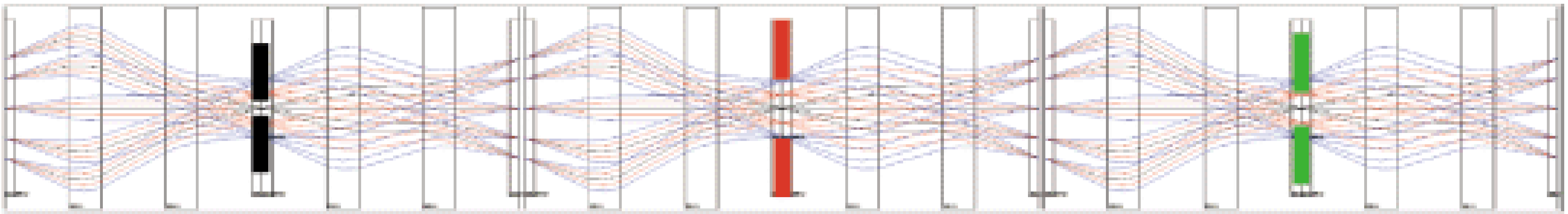
- **Proton transport**
  - **Continuous-energy physics up to 50 GeV**
  - **Direct tracking through magnetic fields**
  - **COSY-map tracking through magnetic fields**
- **Many additional particle types**

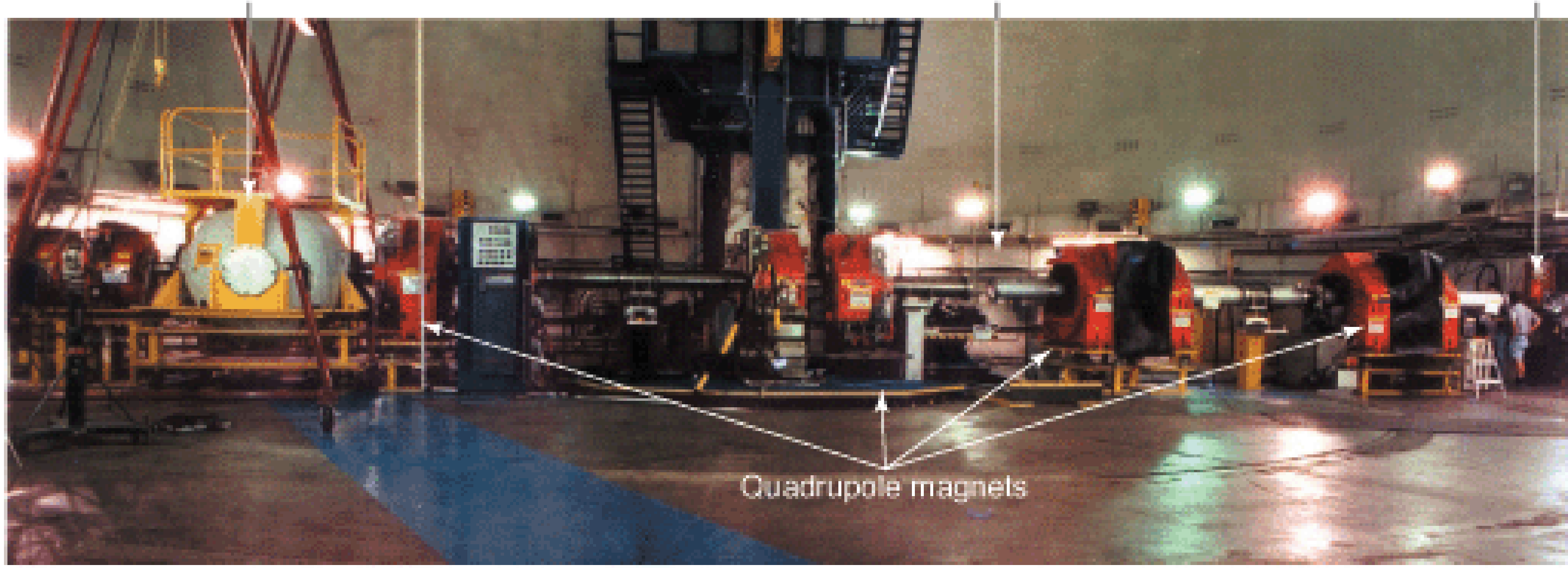
- **ENDF/B-VII** (Data Team)
- **Improved electron transport**
- **Automated variance reduction, using deterministic adjoint**
- **Isotopic source**
- **Criticality**
  - **Stationarity diagnostics (relative entropy)**
  - **Dominance ratio**
  - **Perturbation theory – source shape effects**
  - **Fission neutron multiplicity**
  - **Fission matrix**
- **Continuously varying material properties & tallies**
- Etc.

Proton Radiography

- **For many experiments being conducted now at LANL & BNL, high-energy proton beams are directed at test objects to produce radiographic images**
  - **LANL: 800 MeV proton beams**
  - **BNL: 24 GeV proton beams**
  - **Proposed: 50 GeV proton beams**
- **Proton beams are collimated & focused by magnetic lenses**
- **Both the design of the experiments & analysis of results are carried out using MCNP6, the latest LANL development version of MCNP**
  - **All MCNP5 features plus:**
  - **Continuous-energy proton physics up to 50 GeV**
  - **Models for multiple Coulomb scatter, nuclear elastic scatter, etc.**
  - **Direct tracking of protons through magnetic fields**
  - **COSY-map tracking of protons through magnetic fields**
  - **Many additional particle types being added to account for background**

Proton Radiography

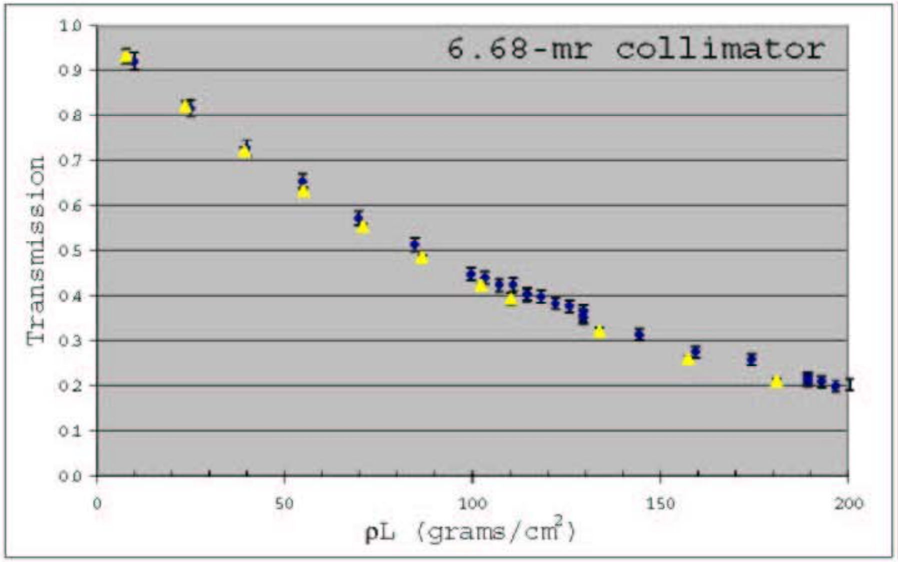


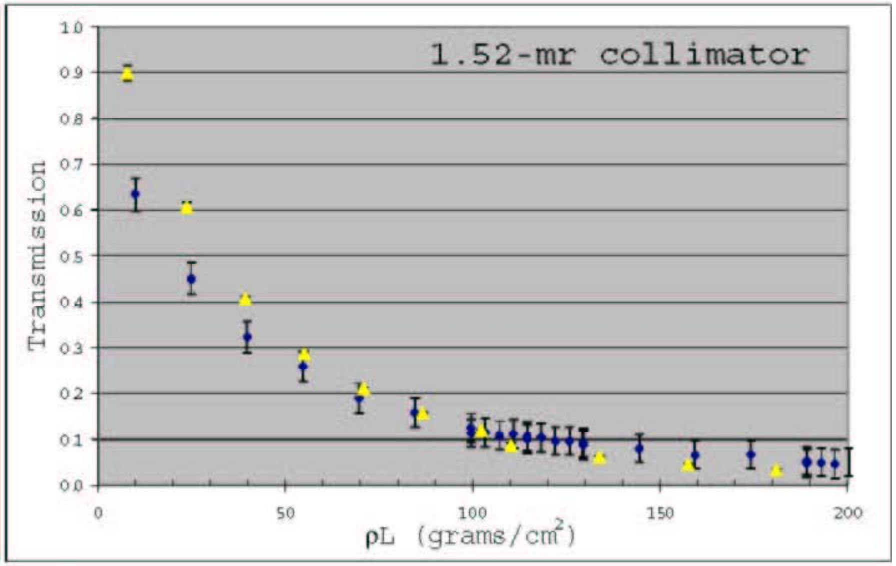


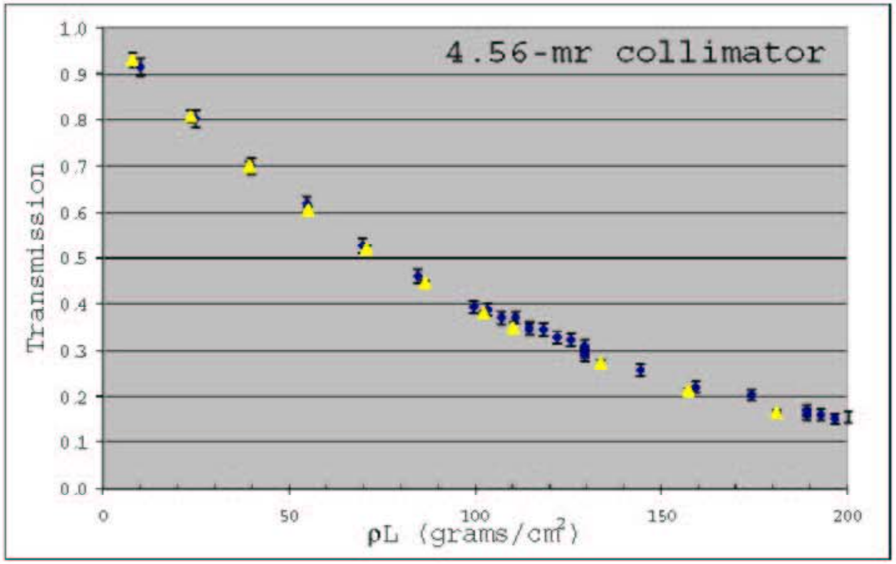
Explosive proton radiography experiments are conducted at the Los Alamos Neutron Science Center facility. In these experiments, a proton beam traveling inside a tube penetrates a target placed in a spherical vessel (left) to contain the explosion. Quadrupole magnets (orange) focus the scattered protons onto imaging detectors. This particular setup uses three imaging stations, including one installed in front of the target to examine the profile of the incoming proton beam. Collimators are located inside the beam tube.

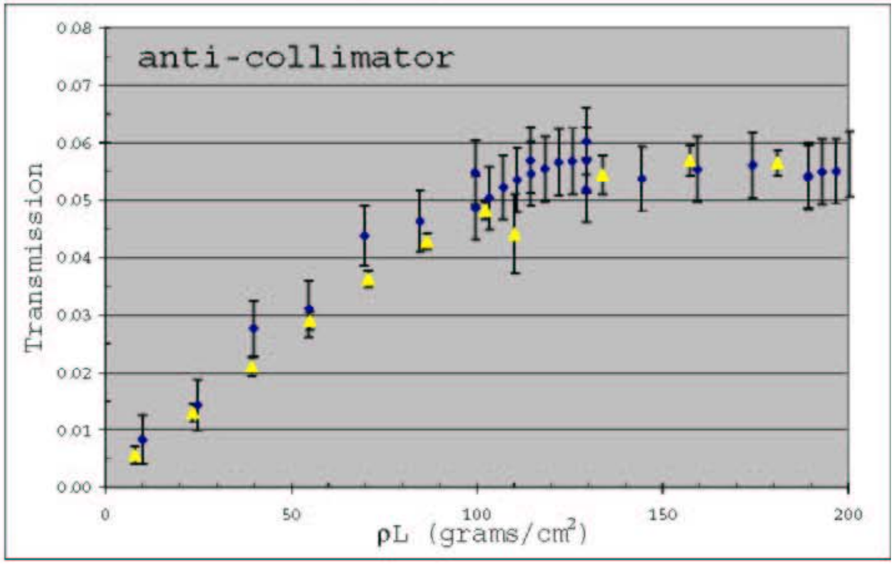
Brookhaven Experiments

Iron target: Blue = data, Yellow = MCNP6 simulation.

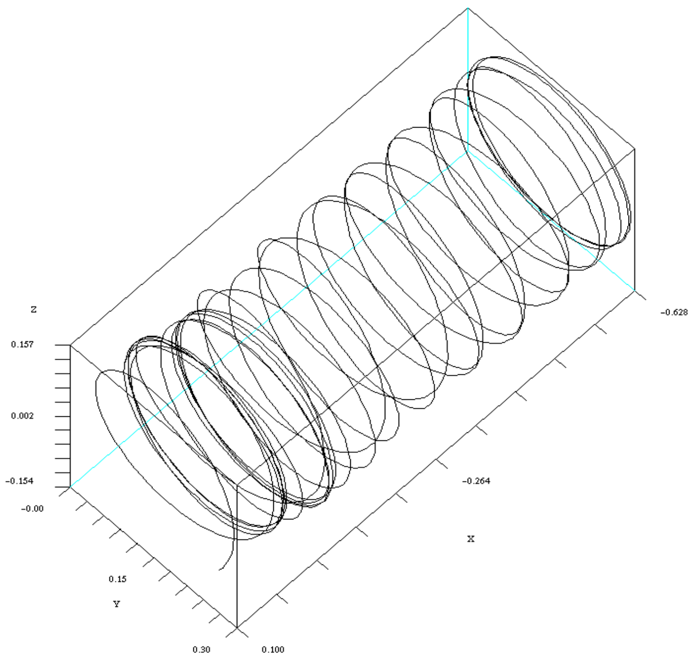








Proton in Air & Constant B Field – No Energy Straggling



Proton in Air & Constant B Field – With Energy Straggling